

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 3.34 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.20e-01

**Confidence level:** 7.67e-01

## Nearest Neighbors from the Training Set

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Methanol

**Measured:** 2.75

**Predicted:** 2.76

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Ethanol

**Measured:** 1.58

**Predicted:** 2.24

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Ethyleneimine

**Measured:** 6.03

**Predicted:** 4.17

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Thioacetamide

**Measured:** 6.03

**Predicted:** 6.43

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1-Propanol

**Measured:** 3.02

**Predicted:** 4.69